Maximal violation of tight Bell inequalities for maximal high-dimensional entanglement

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(Dated: July 30, 2009)

We propose a Bell inequality for high-dimensional bipartite systems obtained by binning local measurement outcomes and show that it is tight. We find a binning method for even d-dimensional measurement outcomes for which this Bell inequality is maximally violated by maximally entangled states. Furthermore we demonstrate that the Bell inequality is applicable to continuous variable systems and yields strong violations for two mode squeezed states.

PACS numbers: 03.65.Ud, 03.65.Ta, 03.67.-a, 42.50.-p

The incompatibility of quantum non-locality with local-realistic (LR) theories is one of the most remarkable aspects of quantum theory. LR theories impose constraints on the correlations between measurement outcomes on two separated systems which are described by Bell inequalities (BIs) [1]. It was shown that BIs are violated by quantum mechanics in the case of entangled states. Therefore BIs are of great importance for understanding the conceptual foundations of quantum theory and also for investigating quantum entanglement. Since the first discussion of quantum non-locality by Einstein-Podolski-Rosen (EPR) a great amount of relevant work has been done and numerous versions of BIs have been proposed [1, 2, 3, 4, 5, 6, 7, 8, 9, 10, 11, 12, 13].

For bipartite 2-dimensional systems the CHSH Bell-type inequality [3] has the desirable property of only being maximally violated for a maximally entangled state. The CHSH inequality divides the space of correlations between measurement outcomes by defining a hyperplane. Since a facet of the polytope defining the region of LR correlations lies in this hyperplane the CHSH inequality is tight. This means that any violation of LR theories occurring on this particular facet is indicated by the CHSH inequality [4]. Tightness is a desirable property since only sets of tight BIs can provide necessary and sufficient conditions for the detection of pure state entanglement. There are still many open questions regarding the generalization of BIs to complex quantum systems [2]. For example, BIs for bipartite high-dimensional systems as e.g. that proposed by Collins *et al.* [5] are either not maximally violated by maximal entanglement [6] or as in the case of Son *et al.* [7] were shown to be non-tight [8].

In the case of continuous variable systems there is so far no known BI formulated in phase space which is maximally violated by the EPR state – the maximally entangled state associated with position and momentum [9]. Although Banaszek and Wodkievicz (BW) showed how to demonstrate non-locality in phase space [10] their BI is not maximally violated by the EPR state [11]. Another approach using pseudospin operators was shown to yield maximal violation for the EPR state [12]. However, finding measurable local observables to realise this approach is challenging. Due to the lack of any known BI providing answers to these questions we still have no clear understanding of nonlocal properties of high-dimensional systems and their relation to quantum entanglement.

In this paper we present a BI for even d-dimensional bipartite quantum systems which, in contrast to previously known BIs, fulfills the two desirable properties of being tight and being maximally violated by maximally entangled states. These properties are essential to investigate quantum non-locality appropriately and for consistency with the 2-dimensional case. We call BIs fulfilling these properties *optimal BIs* throughout this paper. Then we extend optimal BIs to continuous variable systems and demonstrate strong violations for properly chosen local measurements.

Optimal Bell inequality–We begin by briefly introducing the generalized formalism for deriving BIs for arbitrary d-dimensional bipartite systems [8]. Suppose that two parties, Alice and Bob, independently choose one of two observables $\hat{A}_1$ or $\hat{A}_2$ for Alice, and $\hat{B}_1$ or $\hat{B}_2$ for Bob. Possible measurement outcomes are denoted by k_a for $\hat{A}_a$ and l_a for $\hat{B}_b$ with $a, b = 1, 2$, where $k_a, l_b \in V \equiv \{0, 1, ..., d-1\}$. A general Bell function is then written as [8]

$$\mathcal{B} = \sum_{a,b=1}^{2} \sum_{k_a,l_b=0}^{d-1} \epsilon_{ab}(k_a, l_b) P_{ab}(k_a, l_b), \qquad (1)$$

where $P_{ab}(k_a, l_b)$ is the joint probability for outcomes k_a and l_b, and $\epsilon_{ab}(k_a, l_b)$ are their weighting coefficients (here assumed to be real). For local-realistic (LR) systems each probabilistic expectation of $\mathcal{B}$ is a convex combination of all possible deterministic values. It can thus not exceed the maximal deterministic expectation value given by

$$\mathcal{B}_{\rm LR}^{\max} = \max_{C} \Bigg\{ \sum_{a,b=1}^{2} \epsilon_{ab}(k_a, l_b) \Bigg\}, \qquad (2)$$

where $C \equiv \{(k_1, k_2, l_1, l_2) | k_1, k_2, l_1, l_2 \in V\}$ is the set of all possible outcome configurations. A quantum state

violates local realism if its expectation value exceeds the bound $\mathcal{B}_{\rm LR}^{\max}$. The flexibility in choosing the coefficients $\epsilon_{ab}(k_a, l_b)$ allows the derivation of all previously known BIs [8] from Eq. (1), e.g. those proposed by Collins *et al.* [5] and by Son *et al.* [7]. Moreover, we can construct new BIs by properly choosing coefficients $\epsilon_{ab}(k_a, l_b)$. Our aim is to find optimal BIs which fulfil the following conditions:

(C1) The BI is tight i.e. it defines a facet of the polytope separating LR from non-local quantum regions in correlation or joint probability space.

(C2) The BI is maximally violated by a maximally entangled state. For each bipartite d-dimensional maximally entangled state there exists a basis $|j\rangle$ with $j = 0, \cdots, d-1$ in which this state reads $|\psi_d^{\max}\rangle = \sum_{j=0}^{d-1} |jj\rangle/\sqrt{d}$.

As a general method, one could choose the coefficients $\epsilon_{ab}(k_a, l_b)$ freely and examine whether the resulting BI satisfies the conditions (C1) and (C2). Here we instead propose a method which restricts this choice and is guaranteed to give tight BIs. We assume that the coefficients are products of arbitrary binning functions defined by each party as

$$\zeta_R(k) = \begin{cases} +1 & \text{if outcome } k \in R, \\ -1 & \text{otherwise,} \end{cases} \tag{3}$$

where R is an arbitrarily chosen subset of all possible outcomes, i.e. $R \subset V$. The coefficients are then given by

$$\begin{aligned} \epsilon_{11} = \zeta_{R_1}(k_1)\zeta_{S_1}(l_1),\ \epsilon_{12} = \zeta_{R_1}(k_1)\zeta_{S_2}(l_2), \\ \epsilon_{21} = \zeta_{R_2}(k_2)\zeta_{S_1}(l_1),\ \epsilon_{22} = -\zeta_{R_2}(k_2)\zeta_{S_2}(l_2), \end{aligned} \tag{4}$$

where R_a and S_b are subsets of the outcomes of $\hat{A}_a$ and $\hat{B}_b$, respectively. From Eq. (2) we find the LR upper bound $\mathcal{B}_{\rm LR}^{\max} = 2$.

We first show that any BI derived by this method is tight. The extremal points of the polytope separating LR and non-local quantum mechanical correlations are associated with all deterministic configurations C. They are described by $4d^2$ dimensional linearly independent vectors $\mathbf{G}_{k_1,k_2,l_1,l_2} = (\mathbf{e}_{k_1} \otimes \mathbf{e}_{l_1}) \oplus (\mathbf{e}_{k_1} \otimes \mathbf{e}_{l_2}) \oplus (\mathbf{e}_{k_2} \otimes \mathbf{e}_{l_1}) \oplus (\mathbf{e}_{k_2} \otimes \mathbf{e}_{l_2})$, where $\mathbf{e}_k$ is the d-dimensional vector whose k-th component is 1 and all other components are zero. The interior points of the polytope are given by convex combinations of these extremal points and represent the region accessible to LR theories. We now only consider extremal points associated with configurations giving the maximal LR value $\mathcal{B}_{\rm LR}^{\max}$ and denote their number by M. For a polytope defined in $4d^2$ dimensions at least $4d(d-1)$ linearly independent vectors are required to define a facet. Therefore, if $M \geq 4d(d-1)$ the extremal points yielding $\mathcal{B}_{\rm LR}^{\max}$ define a facet of the polytope distinguishing LR from non-local quantum mechanical correlations [4]. We assume the number of elements in the sets R_1, R_2, S_1, S_2 to be n_1, n_2, m_1, m_2, respectively, where $0 \leq n_1, n_2, m_1, m_2 \leq d-1$. We then count the number of configuration giving $\mathcal{B}_{\rm LR}^{\max}$ and find $M = d^2(d^2 - d(n_1+m_1) + n_1(m_1+m_2) + n_2(m_1-m_2)) \geq 4d(d-1)$. Therefore all BIs obtained by this method are tight, i.e. they satisfy condition (C1). Note that any loss of elements in binned subsets may cause them to become non-tight.

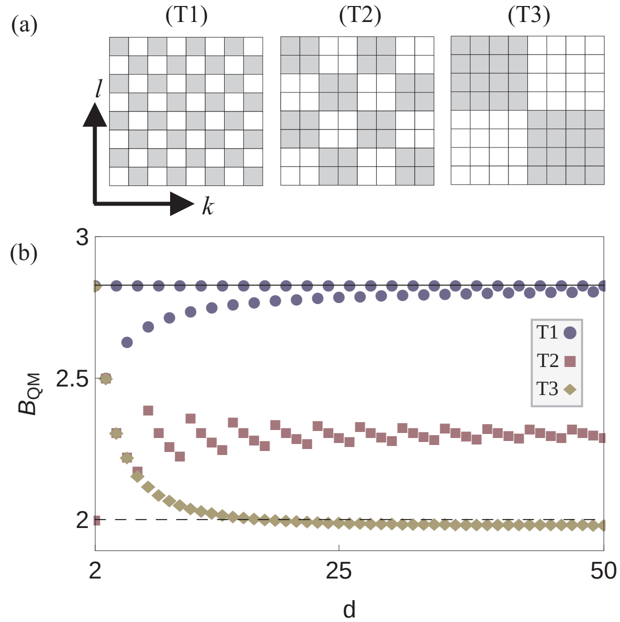

FIG. 1: (a) The coefficient distributions of BIs (T1), (T2), and (T3) for $d = 8$ are shown with weighting +1 (white for ϵ_{11},ϵ_{12},ϵ_{21} and grey for ϵ_{22}) and -1 (grey for ϵ_{11},ϵ_{12},ϵ_{21} and white for ϵ_{22}) in outcome space. (b) Quantum expectation values $\mathcal{B}_{\rm QM}$ of (T1), (T2), and (T3) are plotted. As d increases, the expectation value of (T1) reaches the bound $2\sqrt{2}$ (solid line), while that of (T2) approaches $2.31 < 2\sqrt{2}$ and that of (T3) decreases below the local-realistic upper bound 2 (dashed line).

We now discuss the maximal violation condition (C2) by considering three different tight BIs obtained via the above method. The corresponding choices of the coefficients ϵ_{ab} for $d = 8$ are schematically shown in Fig. 1(a): (T1) is the sharp binning type which can be realised if all outcomes are identifiable with perfect measurement resolution. The elements of the subsets are given as the even-numbers, i.e. $R_1 = R_2 = S_1 = S_2 = \{0, 2, 4, ...\}$ so that the coefficients ϵ_{ab} have an alternating weight $+1$ or -1 when an outcome changes by one. (T2) is associated with unsharp binning resolution and can be used to model imperfect measurement resolution. The subsets are chosen as $R_1 = R_2 = S_1 = S_2 = \{\forall k | k \equiv 0, 1 (\text{mod } 4)\}$ where $k \equiv 0, 1 (\text{mod } 4)$ indicates that k is congruent to 0 or 1 modulo 4. The coefficients ϵ_{ab} alternate between $+1$ and -1 for every 2 outcomes. In type (T3) the measurement results are classified into two divided regions by the mean outcome $[d/2]$, where $[x]$ denotes the integer part of x. The subsets are chosen as $R_1 = R_2 = S_1 = S_2 = \{\forall k | 0 \leq k < [d/2]\}$. These three types of binning correspond to different capabilities in carrying out measurements on d-dimensional systems. Their properties will yield useful

insights for testing BIs in high dimensional and continuous variable systems.

We examine quantum violations of (T1), (T2) and (T3) by the maximally entangled state $|\psi_d^{\max}\rangle$ with increasing dimension d. The measurements $\hat{A}_a$ and $\hat{B}_b$ are performed in the bases $|a,k\rangle = (1/\sqrt{d})\sum_{j=0}^{d-1}\omega^{(k+\alpha_a)j}|j\rangle$ and $|b,l\rangle = (1/\sqrt{d})\sum_{j=0}^{d-1}\omega^{(l+\beta_b)j}|j\rangle$, obtained by quantum Fourier transformation and phase shift operations on $|j\rangle$. Here $\omega = \exp(2\pi i/d)$, and α_a and β_b are phase factors differentiating the observables of each party $\hat{A}_a$ and $\hat{B}_b$, respectively. The expectation value of the Bell function is then given by

$$\mathcal{B}_{\rm QM} = \sum_{a,b=1}^{2}\sum_{k,l=0}^{d-1}\frac{\epsilon_{ab}(k,l)}{2d^3\sin\left[\frac{\pi}{d}(k+l+\alpha_a+\beta_b)\right]}. \qquad (5)$$

As shown in Fig. 1(b), the expectation values of (T1) for even-dimensions are $2\sqrt{2}$, and those for odd-dimensions tend towards $2\sqrt{2}$ with increasing d. This is the upper bound for quantum mechanical correlations which we show by defining a Bell operator as $\hat{\mathcal{B}} = \sum_{a,b}\sum_{k,l}\epsilon_{ab}(k,l)|a,k\rangle\langle a,k|\otimes|b,l\rangle\langle b,l|$. From Eq. (4), $\hat{\mathcal{B}}^2 = 4\mathbb{1}_d\otimes\mathbb{1}_d + [\hat{P}_1,\hat{P}_2]\otimes[\hat{Q}_2,\hat{Q}_1]$ where $\hat{P}_a = \sum_k \zeta_{R_a}(k)|a,k\rangle\langle a,k|$, $\hat{Q}_b = \sum_l \zeta_{S_b}(l)|b,l\rangle\langle b,l|$ and $\mathbb{1}_d$ is the d-dimensional identity operator. Since $\|[\hat{P}_1,\hat{P}_2]\| \le \|\hat{P}_1\hat{P}_2\| + \|\hat{P}_2\hat{P}_1\| \le 2\|\hat{P}_1\|\|\hat{P}_2\| = 2$ and likewise for $\|[\hat{Q}_2,\hat{Q}_1]\|$ where $\|\cdot\|$ indicates the supremum norm, we finally obtain $\|\hat{\mathcal{B}}^2\| \le 8$, or $\|\hat{\mathcal{B}}\| \le 2\sqrt{2}$.

We calculate the quantum mechanical expectation value of $\hat{\mathcal{B}}$ for BI (T1) by writing the coefficients as $\epsilon_{11} = \epsilon_{12} = \epsilon_{21} = (-1)^{k+l}$ and $\epsilon_{22} = -(-1)^{k+l}$. For even d we use $\sum_{k,l=0}^{d-1}(-1)^{k+l}/2d^3\sin\left[\frac{\pi}{d}(k+l+\alpha_a+\beta_b)\right] = \cos\pi(\alpha_a+\beta_b)$ and find the expectation value

$$\begin{aligned}\mathcal{B}_{\rm QM} &= \cos\pi(\alpha_1+\beta_1)+\cos\pi(\alpha_1+\beta_2)\\ &\quad+\cos\pi(\alpha_2+\beta_1)-\cos\pi(\alpha_2+\beta_2). \qquad (6)\end{aligned}$$

This expression also holds approximately for sufficiently large odd d. Thus we obtain $\mathcal{B}_{\rm QM} = 2\sqrt{2}$, i.e. the maximal quantum upper bound, for $\alpha_1 = 0$, $\alpha_2 = 1/2$, $\beta_1 = -1/4$, and $\beta_2 = 1/4$. Figure 1(b) also shows the maximal expectation values of (T2) which are smaller than $2\sqrt{2}$ and approach ≈ 2.31 with increasing d. The maximal expectation values of (T3) decrease below the local-realistic upper bound 2 with increasing d.

These results show that (T1) is an optimal BI for even d which satisfies conditions (C1) and (C2). The optimal correlation operator is then written as $\hat{E}_{ab} = \hat{\Pi}_a\otimes\hat{\Pi}_b$. with the local measurement $\hat{\Pi}_a = \sum_{k=0}^{d-1}(-1)^k|a,k\rangle\langle a,k|$. Finally, we obtain the optimal BI

$$\mathcal{B} = E_{11}+E_{12}+E_{21}-E_{22} \le 2, \qquad (7)$$

where $E_{ab} = \langle\hat{E}_{ab}\rangle = \sum_{k,l}(-1)^{k+l}P_{ab}(k,l)$ is the correlation function. Note that for $d=2$ Eq. (7) is equivalent to the CHSH inequality [3]. We have thus shown that the perfect sharp binning of arbitrary even dimensional outcomes (T1) provides an optimal BI, while the other binning methods (T2) and (T3) tend to neglect quantum properties and do not show maximal violation for maximally entangled states.

Continuous variable systems–We extend the optimal BI (T1) to a continuous variable system and calculate its violation by a two-mode squeezed state (TMSS). This state can, for instance, be realised by non-degenerate optical parametric amplifiers [13] in photonic systems. It is written as $|{\rm TMSS}\rangle = {\rm sech}r\sum_{n=0}^{\infty}\tanh^n r|n,n\rangle$ where $r>0$ is the squeezing parameter and $|n\rangle$ are the number states of each mode. In the infinite squeezing limit $r\to\infty$, this becomes the normalized EPR state [10].

When directly following the procedure of the finite dimensional case two problems arise: First, we obtain the local measurement basis by applying the quantum Fourier transformation to $|n\rangle$. This is equivalent to the phase states $|\theta\rangle = (1/\sqrt{2\pi})\sum_{n=0}^{\infty}\exp(in\theta)|n\rangle$ which are not orthogonal and not eigenstates of any hermitian observable. Therefore no precise phase measurement can be carried out. Second, a naive extension of the sharp binning method to the continuous case is impossible. Note that any coarse-grained measurement tends to lose quantum properties [14] and lead to non-tight BI tests. From the above results for unsharp and regional binning we also do not expect strong violations by these methods for the continuous variable system.

Let us consider the Pegg-Barnett phase state formalism [15]. We approximate the quantum phase by an orthonormal set of phase states in a $s+1$-dimensional truncated space $|\theta,k\rangle = (1/\sqrt{s+1})\sum_{n=0}^{s}\exp(in\theta_k)|n\rangle$ where $\theta_k = \theta+2\pi k/(s+1)$ and $k = 0,1,...,s$. Note that s is a cutoff parameter (assumed here to be an odd number) and in the limit $s\to\infty$ there exists a θ_k arbitrarily close to any given continuous phase. The correlation operator can then be written as $\hat{E}(\theta,\phi) = \hat{\Pi}(\theta)\otimes\hat{\Pi}(\phi)$ using the *phase parity operator* $\hat{\Pi}(\theta) = \sum_{k=0}^{s}(-1)^k|\theta,k\rangle\langle\theta,k|$.

We consider a truncated TMSS $|\psi_s\rangle = ({\rm sech}r/\sqrt{1-\tanh^{2s+2}r})\sum_{n=0}^{s}\tanh^n r|n,n\rangle$ which tends to the $s+1$-dimensional maximally entangled state for $r\to\infty$ and to the TMSS for an infinite cutoff, $s\to\infty$. The preparation of this state can for instance be achieved by the optical state truncation method [16].

The expectation value of the Bell operator is given by

$$\begin{aligned}\mathcal{B}_{\rm QM} &= \langle\psi_s|\hat{E}(\theta,\phi)+\hat{E}(\theta,\phi')+\hat{E}(\theta',\phi)-\hat{E}(\theta',\phi')|\psi_s\rangle\\ &= 4\sqrt{2}\frac{\tanh^{\frac{s+1}{2}}r}{1+\tanh^{s+1}r}, \qquad (8)\end{aligned}$$

when $\theta = 0$, $\theta' = \pi/(s+1)$, $\phi = -\pi/(2s+2)$, and $\phi' = \pi/(2s+2)$. Fig. 2(a) shows its monotonic increase against the squeezing rate r for different cutoff parameters s. For any finite s and $\delta>0$ there exists a squeezing parameter r above which $\mathcal{B}_{\rm QM} \ge 2\sqrt{2}-\delta$. The required squeezing for this violation is $r \ge \frac{1}{2}\ln[(1+f(s,\delta))/(1-f(s,\delta))]$ where $f(s,\delta) = [(2\sqrt{2}-\sqrt{4\sqrt{2}\delta-\delta^2})/(2\sqrt{2}-\delta)]^{2/(s+1)}$.

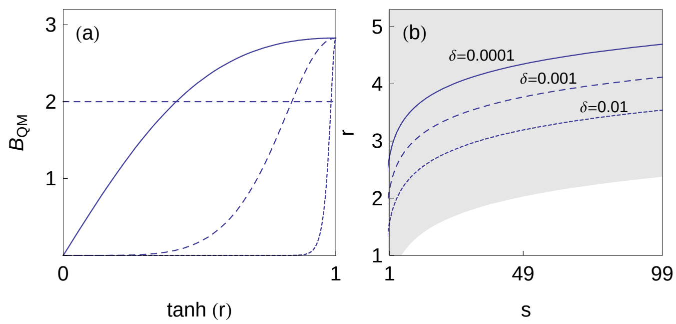

FIG. 2: (a) Expectation values of the Bell operator for truncated TMSS with cutoff parameters $s = 1$ (solid), $s = 9$ (dashed), and $s = 99$ (dotted). (b) The shaded region indicates the values of r for which the BI is violated; a violation better than $\mathcal{B}_{\rm QM} \geq 2\sqrt{2} - \delta$ occurs above the curves shown for $\delta = 0.01$ (dotted), $\delta = 0.001$ (dashed), and $\delta = 0.0001$ (solid).

The shaded region in Fig. 2(b) indicates the values of r for which the BI is violated $\mathcal{B}_{\rm QM} \geq 2$ and a violation better than $\mathcal{B}_{\rm QM} \geq 2\sqrt{2} - \delta$ occurs for values of r above the corresponding curves for different δ. Violations arbitrarily close to the maximum value $2\sqrt{2}$ can thus be achieved by sufficiently strongly squeezed states for any finite value of s with $r \to \infty$ corresponding to the EPR state. Remarkably, this is in contrast to previous types of BIs which were not able to get arbitrarily close to this bound for the EPR state. However, we should note that for large s one here again faces difficulties in performing precise measurements due to the indistinguishability of two local measurements as $\pi/(s+1) \to 0$ for large s.

Finally, we discuss the relation of our optimal BI with the BW inequality proposed in [10]. There, local measurements are performed in the basis obtained by applying a Glauber displacement operator $\hat{D}(\alpha)$ on the number states $|n\rangle$. The measurement basis is written as $|\alpha, n\rangle = \hat{D}(\alpha)|n\rangle$ with α an arbitrary complex number. The displaced number operator is defined as $\hat{n}_\alpha \equiv \hat{D}(\alpha)\hat{n}\hat{D}^\dagger(\alpha)$. Since $\hat{n}_\alpha|\alpha, n\rangle = n|\alpha, n\rangle$, the correlation operator is given by $\hat{E}(\alpha, \beta) = \hat{\Pi}(\alpha) \otimes \hat{\Pi}(\beta)$, where $\hat{\Pi}(\alpha) = \sum_{n=0}^{\infty}(-1)^n|\alpha, n\rangle\langle\alpha, n|$ is the displaced parity operator. Using this notation the BW inequality becomes equivalent to Eq. (7), which shows that it is a tight BI for continuous variable systems. However, the maximal expectation value of the BW inequality was shown to be $2.32 < 2\sqrt{2}$ [11], while our type of BI asymptotically reaches the bound $2\sqrt{2}$. This shows that the optimal measurement bases for this non-locality test are obtained by a quantum Fourier transformation on the standard bases [17], i.e. each of them is mutually unbiased to the standard basis. This may also provide a useful insight about the optimality of measuring in mutually unbiased bases for cases with more than two local measurements [18].

Conclusions–We derived, for the first time, a BI in even d-dimensional bipartite systems which is maximally violated by maximal entanglement and is also tight. These are desirable properties for BIs in high-dimensional systems [2, 8]. Our BI is found by perfectly sharp binning of the local measurement outcomes. It can be used for testing quantum non-locality for high dimensional systems, for instance it coincides with the result for heteronuclear molecules by Milman *et al.* [19]. Furthermore, we extended our studies to continuous variable systems and demonstrated strong violations asymptotically reaching the maximal bound $2\sqrt{2}$ for truncated TMSSs by parity measurements in the Pegg-Barnett phase basis. This provides a theoretical answer to the question of how maximal violations of BIs can be demonstrated for the EPR states in phase space formalism [9]. In the future we will investigate the susceptibility of violations of our BIs to measurement imperfections. In this context it will also be valuable to search for additional optimal BIs comparing their properties and extending optimal BIs to multipartite systems.

We thank J. Lee, I. A. Walmsley and U. Dorner for valuable discussions. This work was supported by the EU through the STREP project OLAQUI and by the UK EPSRC through projects QIPIRC (GR/S82176/01) and EuroQUAM (EP/E041612/1).

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